Multiphase Flows and Hyperbolic PDEs
-
A Mixture of Topics

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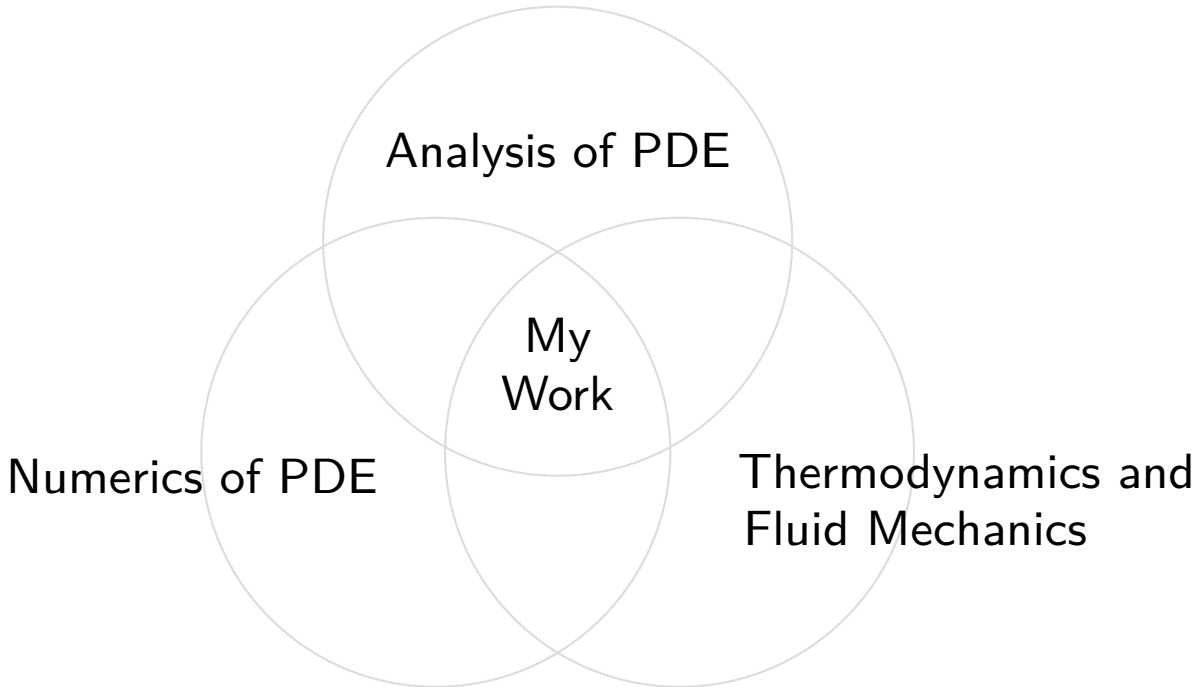
EMS TAG Mixtures Meeting - Prague 2025

The main focus lies on the description and understanding of the dynamics of a liquid/vapor flow of a single substance (e.g. water).



Results for a sharp interface model

Sharp Interface Two Phase Flow

Present sharp interface modeling approach:

- *one* set of Euler equations for *both* phases
- assume a sharp (zero thickness) interface
- clearly distinguish the phases and use appropriate *EOS*
- consider a compressible fluid
- allow non-equilibrium states, i.e. different pressures at the interface

Isothermal Euler Equations

Brief summary of the problem setting:
We consider the 1-D isothermal Euler equations for $(t, x) \in (0, \infty) \times \mathbb{R}$

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial x} &= 0, \\ \frac{\partial (\rho u)}{\partial t} + \frac{\partial (\rho u^2 + p)}{\partial x} &= 0. \end{aligned} \tag{E-Eq-T}$$

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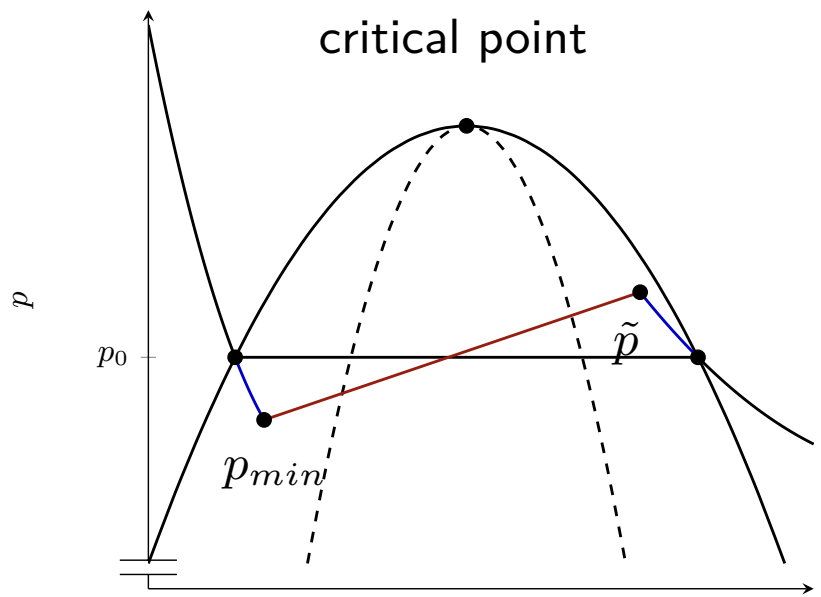
The phases are distinguished by their phase densities and described by their EOS

$$0 \leq \rho_V \leq \tilde{\rho},\ p_V(\rho_V)\ \text{(vapor)} \quad \text{and} \quad \rho_L \geq \rho_{min},\ p_L(\rho_L)\ \text{(liquid)}$$



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The mass transfer is modeled using a kinetic relation determining the mass flux at the interface and which is compatible with the mathematical entropy inequality.

Conditions at the Interface

There exists a unique liquid state for given vapor state satisfying the nonlinear system[1]

$$\begin{aligned} -\rho(u-w) &= z, \\ [\![\rho(u-w)]\!] &= 0, \\ \rho(u-w)\,[\![u]\!] + [\![p]\!] &= 0, \\ z - \tau p_V\,[\![g + e_{kin}]\!] &= 0. \end{aligned}$$

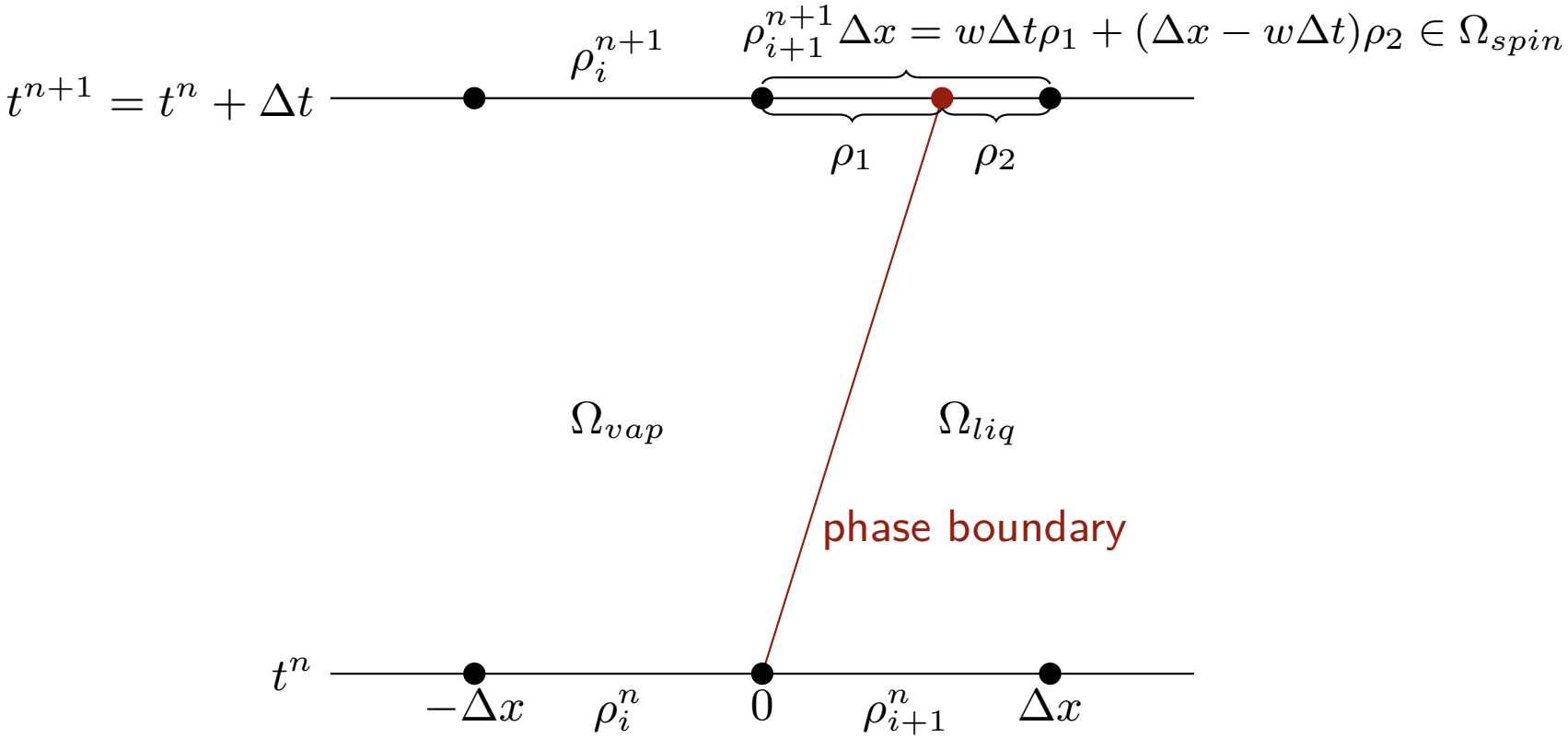
This system can be collapsed into a single nonlinear equation, i.e.

$$[\![p]\!] = -z^2 \left[\!\!\left[\frac{1}{\rho}\right]\!\!\right]$$

[1] Hantke, M. & Thein, F. A general existence result for isothermal two-phase flows with phase transition. *Journal of Hyperbolic Differential Equations* **16,** 595–637. eprint: https://doi.org/10.1142/S0219891619500206 (2019).

Numerics - Main Challenges

- if two adjacent cells belong to the same phase any standard Riemann solver can be used
- we are only interested in the case where two adjacent cells belong to different phases
- due to the solution structure & CFL-condition the phase boundary will lie inside a cell for $w \neq 0$; hence averaging can lead to non-physical states



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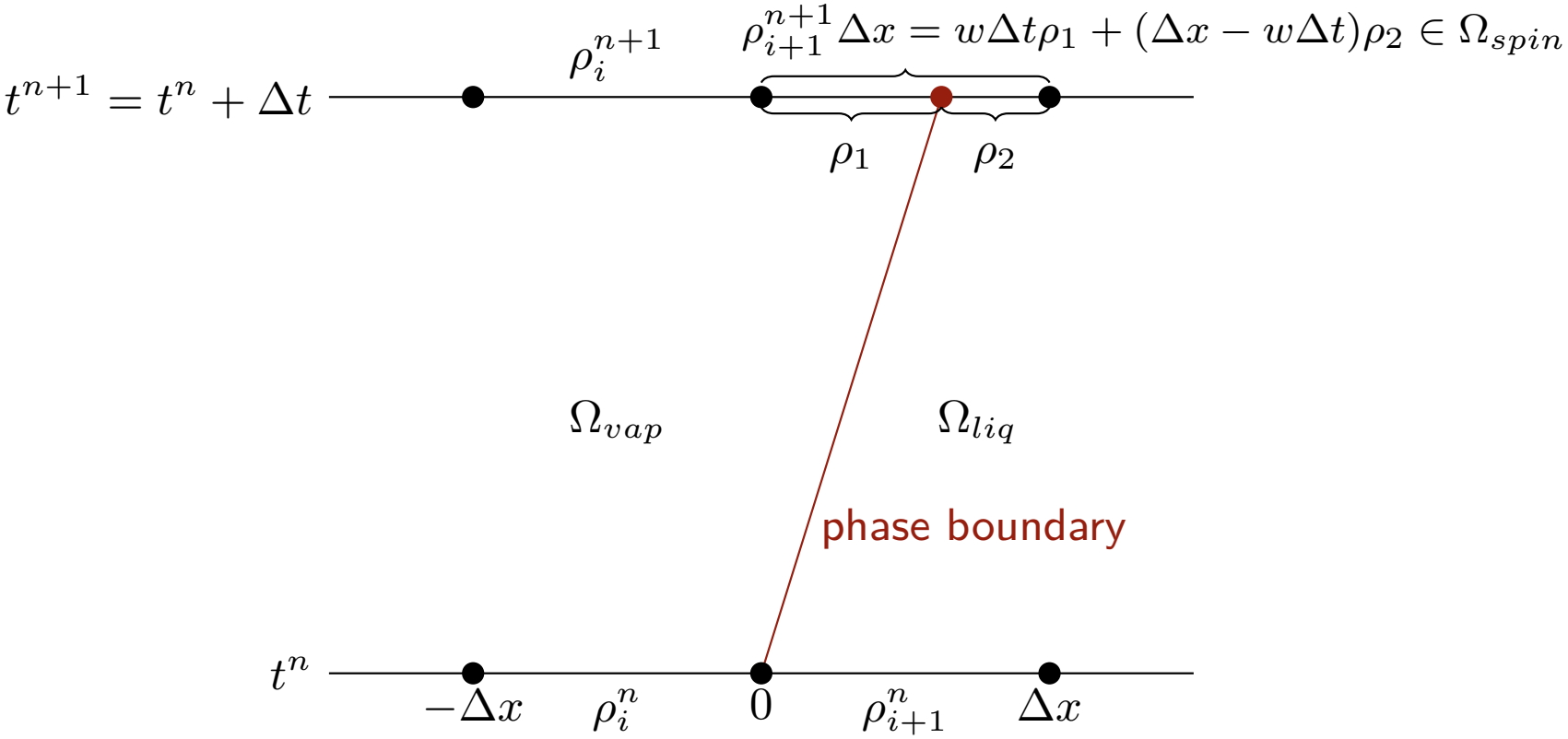


- we need to localize the phase boundary
- we need to calculate the quantities in the star region
- we need to determine the correct flux at the phase boundary
- due to the motion of the phase boundary we will obtain different cell sizes; this affects the time step

Grid Adaption

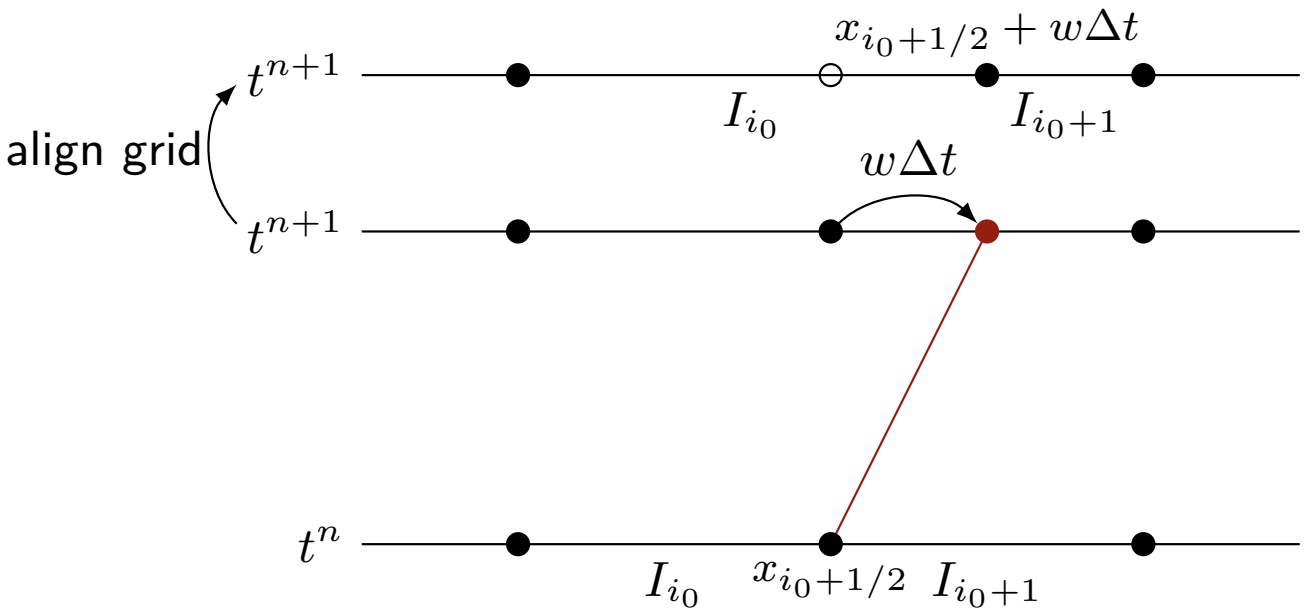


Figure: Align grid to the new position of the phase boundary.

To ensure suited cell sizes split cells which are too large and merge cells which are too small.

Create a new cell of size $(w_{right} - w_{left})\Delta t$ with the obtained state variables:

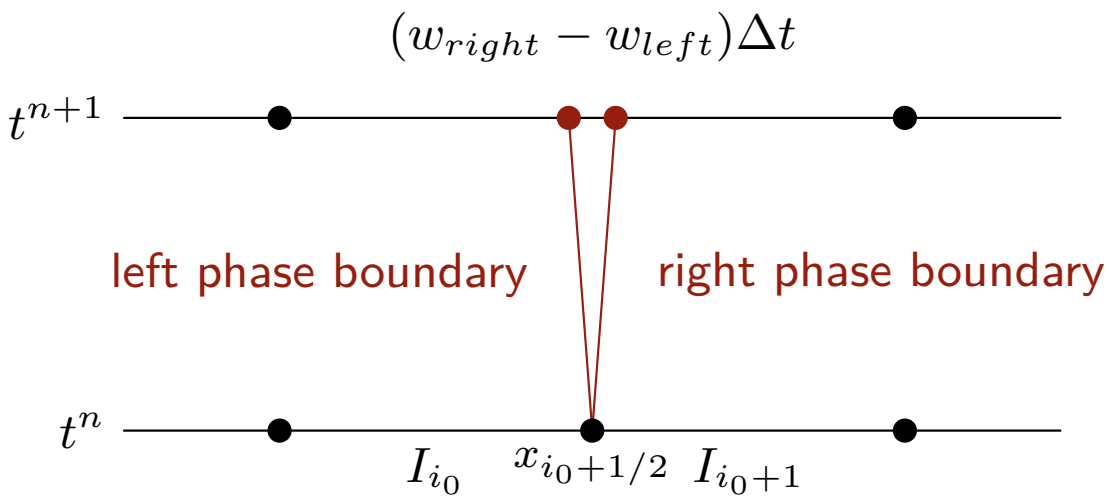
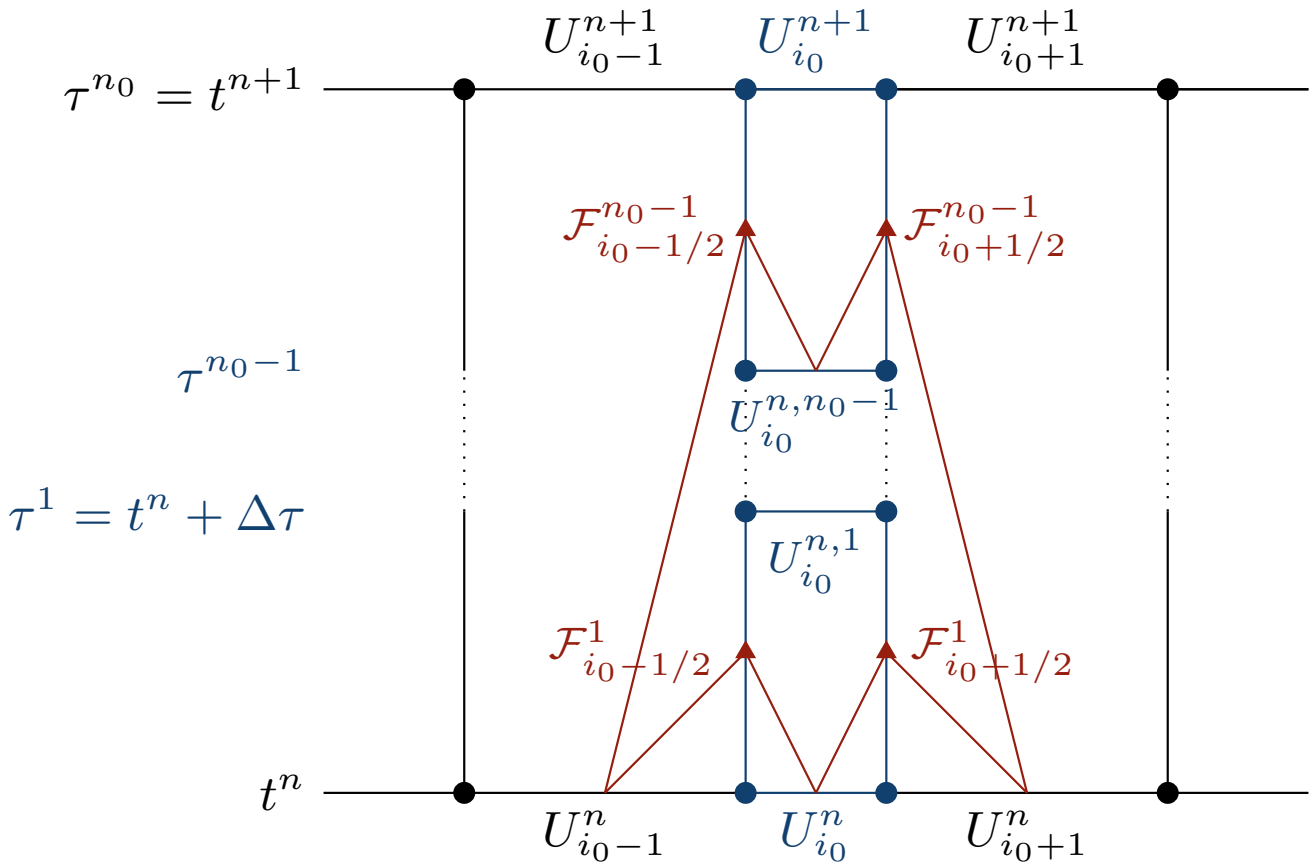


Figure: For initial states that belong to one phase phase creation (i.e., cavitation or nucleation) can occur. In the simulation this results in the creation of a small cell from one time step to the next. This cell must not be merged with its neighbors since they belong to different phases.

Isolated Small Cells - The story so far...

For isolated small cells it is beneficial to use local time stepping, see Müller et al.[2].



Number of small time steps scales with $1/\alpha$!

[2] Müller, S. & Stiriba, Y. Fully Adaptive Multiscale Schemes for Conservation Laws Employing Locally Varying Time Stepping. English. *Journal of Scientific Computing* **30,** 493–531. ISSN: 0885-7474 (2007).

Still, very small cells have a crucial impact on the computational time and a faster method would be beneficial to have. Here we present the results obtained in May and T[3].

[3] May, S. & Thein, F. Explicit implicit domain splitting for two phase flows with phase transition. *Physics of Fluids* **35,** 016108. eprint: https://doi.org/10.1063/5.0131908 (2023).

The Small Cell Problem

For simplicity assume the mesh to be fixed. We denote the cell centroid of cell I_i with x_i and the edges with $x_{i\pm\frac{1}{2}}$. When phase creation occurs the mesh may look like this

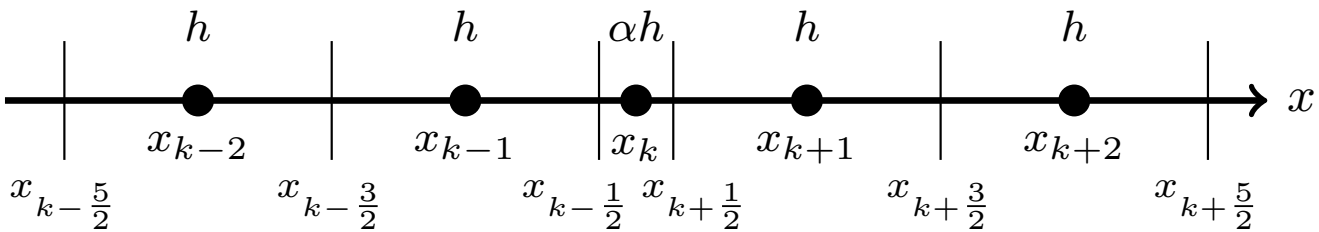


Figure: 1d model problem: equidistant mesh of mesh width h with one small cell (cell I_k) of length αh, $\alpha \in (0, 1]$. Cell I_k corresponds to the creation of a new phase.

In space we use *Godunov's method*.

Explicit Implicit Domain Splitting

We suggest a mixed explicit implicit approach: only treat the neighborhood of the small cell I_k implicit for stability, but treat all the cells away from the small cell explicit to keep the cost low.

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Question: How to change between explicit and implicit time stepping while ensuring conservation and maintaining stability?

For the linear advection equation on cut cell meshes this was investigated by May and Berger[4]: desirable properties are preserved.

[4] May, S. & Berger, M. J. An explicit implicit scheme for cut cells in embedded boundary meshes. *J. Sci. Comput.* **71,** 919–943 (2017).

Explicit Implicit Domain Splitting

In each time step:

1. we first update all cells with indices $i \leq k-2$ and $i \geq k+2$ using a fully explicit update

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2. we then update solution values on cells I_{k-1}, I_k, I_{k+1} using:

$$\mathbf{U}_{k-1}^{n+1} = \mathbf{U}_{k-1}^{n} - \frac{\Delta t}{h}\left[\mathbf{F}_{k-\frac{1}{2}}(\mathbf{U}_{k-1}^{n+1}, \mathbf{U}_{k}^{n+1}) - \mathbf{F}_{k-\frac{3}{2}}(\mathbf{U}_{k-2}^{n}, \mathbf{U}_{k-1}^{n})\right],$$

$$\mathbf{U}_{k}^{n+1} = \mathbf{U}_{k}^{n} - \frac{\Delta t}{\alpha h}\left[\mathbf{F}_{k+\frac{1}{2}}(\mathbf{U}_{k}^{n+1}, \mathbf{U}_{k+1}^{n+1}) - \mathbf{F}_{k-\frac{1}{2}}(\mathbf{U}_{k-1}^{n+1}, \mathbf{U}_{k}^{n+1})\right],$$

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Dual Time Stepping

- In the mixed explicit implicit approach, the implicit time stepping only couples solution values on cells I_{k-1}, I_k, I_{k+1}.
- Update formulae involve non-linear flux functions, in particular Riemann solvers for phase changes $\rightarrow$ solving the resulting implicit system is still non-trivial.

Idea: Use dual time stepping for doing this.

Advantage: No need to differentiate through the Riemann solver and the implementation work for changing a running code from explicit to implicit time stepping is quite small.

Example

Two Phase Flows - Setup

For the isothermal case we model the vapor phase as an ideal gas using the relation

$$p_V = \frac{kT_0}{m}\rho_V,\ m = \frac{2 \cdot 1.0079 + 15.9994}{6.02205 \cdot 10^{26}}\ \text{kg},\ k = 1.380658 \cdot 10^{-23}\ \text{JK}^{-1}$$

where k is the Boltzmann constant and m the mass of a single water molecule. The coefficient τ for the kinetic relation is given by

$$\tau = \frac{1}{\sqrt{2\pi}} \left(\frac{m}{kT_0} \right)^{3/2}.$$

The liquid phase is described using the linear Tait EOS

$$p_L = p_0 + K_0 \left(\frac{\rho_L}{\rho_0} - p_0 \right).$$

All quantities with a subscript zero are saturation quantities at the given temperature T_0 evaluated according to the steam tables in Ref.[5].

[5] Wagner, W. & Kruse, A. *Properties of water and steam: the industrial standard IAPWS-IF97 for the thermodynamic properties and supplementary equations for other properties : tables based on these equations.* ISBN: 9783540643395 (Springer-Verlag, 1998).

Nucleation - Problem

Consider the following initial data

	p_V^-	u_V^-	p_V^+	u_V^+
Initial Data	$70000\,\text{Pa}$	$2.7\,\frac{\text{m}}{\text{s}}$	$70000\,\text{Pa}$	$-2.7\,\frac{\text{m}}{\text{s}}$

	T_0	p_0
Saturation Values	$363.15\,\text{K}$	$70182.360745\,\text{Pa}$

Table: Nucleation Test: Initial Data.

The computation was performed with $C_{CFL} = 0.5$, $h^0 = 10^{-2}\,\text{m}$, $x \in [-2, 2]\,\text{m}$, and $t_{\text{end}} = 5 \cdot 10^{-4}\,\text{s}$. The time step is calculated according to the CFL-condition and the phases are distinguished as before.

Nucleation - Results

- cell size of the liquid phase after its creation is $h_L = 4.429422 \cdot 10^{-9}$ m
  $\rightarrow$ initial $\alpha \sim \mathcal{O}(10^{-7})$
- values for the interface velocities are $w_{\text{left/right}} = \pm 0.000203 \, \frac{\text{m}}{\text{s}}$
  $\rightarrow$ size of liquid cell at time t_{end} is $(w_{right} - w_{left}) \cdot t_{\text{end}} = 2.03 \cdot 10^{-7}$ m.

Nucleation - Results

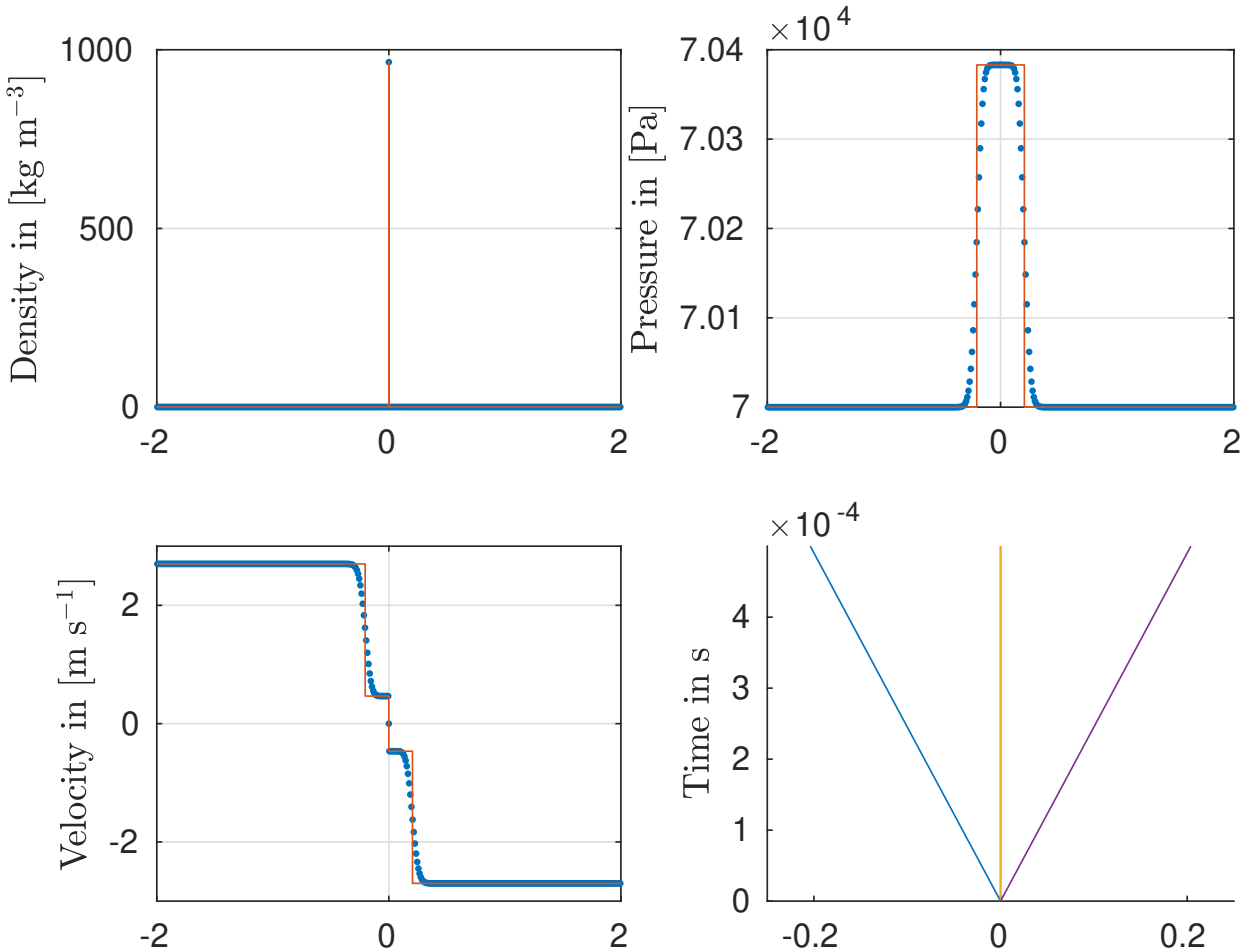

Figure: Nucleation Test: Computed (blue) and exact (red) solution as well as the exact wave structure of the solution showing the outgoing shock waves and the two phase boundaries in the middle of the fan.

Nucleation - Results

	explicits LTS	implicit (DTS)
number of total local iterations	$27'154'016$	$1'367'460$
computation time	9811s	509s

Table: Nucleation Test: Comparison of computational costs.

- 143 large time steps
- explicit LTS needs roughly a factor of 20 more iterations

Some Answers

(i) existence/uniqueness for arbitrary (thermodynamically reasonable) EOS can be shown, see Hantke, T.[6]

(ii) similar results in the adiabatic case *cannot* be expected
→ non-existence result for two phases, see Hantke, T.[7]
→ condensation by compression not possible, see Hantke, T.[8]
→ need for additional quantities and thus loss of self similarity, see Hantke, T.[9]

(iii) numerical results for the isothermal case, including phase creation and an approximation at the interface, see May, T.[10]

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[6] Hantke, M. & Thein, F. A general existence result for isothermal two-phase flows with phase transition. *Journal of Hyperbolic Differential Equations* **16,** 595–637. eprint: https://doi.org/10.1142/S0219891619500206 (2019).

[7] Hantke, M. & Thein, F. On the Impossibility of First-Order Phase Transitions in Systems Modeled by the Full Euler Equations. *Entropy* **21.** ISSN: 1099-4300 (2019).

[8] Hantke, M. & Thein, F. Why condensation by compression in pure water vapor cannot occur in an approach based on Euler equations. *Quart. Appl. Math.* **73,** 575–591 (2015).

[9] Hantke, M. & Thein, F. Singular and selfsimilar solutions for Euler equations with phase transitions. *Bulletin of the Brazilian Mathematical Society, New Series* **47,** 779–786 (2016).

[10] May, S. & Thein, F. Explicit implicit domain splitting for two phase flows with phase transition. *Physics of Fluids* **35,** 016108. eprint: https://doi.org/10.1063/5.0131908 (2023).

Results for a diffuse mixture model

Diffuse Mixture Two Phase Flow

Present diffuse mixture modeling approach:

- *one* set of Euler equations for *each* phase
- assume a mixture of both phases
- coupling of phases via volume fraction $\alpha \in (0, 1)$
- $\rightarrow$ additional transport equation for α
- consider a compressible fluid

Barotropic SHTC Model

We consider the barotropic two fluid model given by the following five equations

$$\begin{aligned}
\frac{\partial \alpha_1 \rho}{\partial t} + \frac{\partial \alpha_1 \rho u}{\partial x} &= 0, \\
\frac{\partial \alpha_1 \rho_1}{\partial t} + \frac{\partial \alpha_1 \rho_1 u_1}{\partial x} &= 0, \\
\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} &= 0, \\
\frac{\partial (\alpha_1 \rho_1 u_1 + \alpha_2 \rho_2 u_2)}{\partial t} + \frac{\partial \left(\alpha_1 \rho_1 u_1^2 + \alpha_2 \rho_2 u_2^2 + \alpha_1 p_1(\rho_1) + \alpha_2 p_2(\rho_2) \right)}{\partial x} &= 0, \\
\frac{\partial (u_1 - u_2)}{\partial t} + \frac{\partial \left(\frac{1}{2} u_1^2 - \frac{1}{2} u_2^2 + \Psi_1(\rho_1) - \Psi_2(\rho_2) \right)}{\partial x} &= 0.
\end{aligned} \tag{1}$$

This model exhibits interesting analytical properties, see Dumbser, Romenski, F.T.[11]

[11] F.T. *et al.* Exact and Numerical Solutions of the Riemann Problem for a Conservative Model of Compressible Two-Phase Flows. *Journal of Scientific Computing* **93,** 83. ISSN: 1573-7691 (2022).

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\end{aligned} \tag{1}$$

Here we introduce as usual the following quantities and relations $i = 1, 2$

volume fraction phase $i \sim \alpha_i$,

density phase $i \sim \rho_i$,

velocity phase $i \sim u_i$,

pressure phase $i \sim p_i(\rho_i)$.

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\end{aligned} \tag{1}$$

The following mixture quantities and saturation relations are used

$$\begin{aligned}
\alpha_1 + \alpha_2 &= 1, \\
\alpha_1 \rho_1 + \alpha_2 \rho_2 &= \rho, \text{ (mixture density)}, \\
\frac{\alpha_i \rho_i}{\rho} &= c_i,\ c_1 + c_2 = 1, \text{ (concentration phase } i), \\
c_1 u_1 + c_2 u_2 &= u, \text{ (mixture velocity)},\ u_1 - u_2 = w, \text{ (relative velocity)}.
\end{aligned}$$

Energy Inequality

The system is endowed with a mathematical entropy inequality. The total energy inequality for the isentropic case reads

$$\sum_{i=1}^{2} \frac{\partial \alpha_i \rho_i \left(e_i + \frac{1}{2}u_i^2\right)}{\partial t} + \frac{\partial \alpha_i \rho_i u_i \left(h_i + \frac{1}{2}u_i^2\right)}{\partial x} \leq 0$$

and for the isothermal case we have

$$\sum_{i=1}^{2} \frac{\partial \alpha_i \rho_i \left(e_i - T s_i + \frac{1}{2}u_i^2\right)}{\partial t} + \frac{\partial \alpha_i \rho_i u_i \left(g_i + \frac{1}{2}u_i^2\right)}{\partial x} \leq 0.$$

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These are the α - weighted sums of the individual phase energies.
The energy is not strictly convex for equilibrium states[11].

[11] Thein, F. The Shizuta - Kawashima Condition for the Barotropic SHTC Two Fluid Model. *XVIII International Conference on Hyperbolic Problems: Theory, Numerics, Applications* (2023).

Rarefaction Wave

In the following we use $\mu, \nu \in \{1, 2\}, \mu \neq \nu$ where $\mu = 1$ for $\boldsymbol{R}_{1\pm}$ and $\mu = 2$ for $\boldsymbol{R}_{2\pm}$. The relations for ρ_μ and u_μ, obtained from the corresponding eigenvector, can be combined to

$$\frac{\mathrm{d}u_\mu}{\mathrm{d}\rho_\mu} = \pm \frac{a_\mu}{\rho_\mu}.$$

Thus we yield the following invariants '

$$\alpha_1 = const., \quad \mathcal{R}_\pm = u_\mu \pm \int \frac{a_\mu}{\rho_\mu} \, \mathrm{d}\rho_\mu, \quad \rho_\nu = const. \quad \text{and} \quad u_\nu = const.$$

Furthermore the slope inside a left rarefaction wave is given by

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \frac{x}{t} = \lambda_{\mu\pm} = u_\mu \pm a_\mu$$

and hence we obtain that the solution inside the rarefaction fan is given by

$$u_\mu = \frac{x}{t} \mp a_\mu \quad \text{and} \quad u_{\mu,R} - u_{\mu,L} \pm \int_{\rho_{\mu,L}}^{\rho_{\mu,R}} \frac{a_\mu}{\rho_\mu} \, \mathrm{d}\rho_\mu = 0.$$

The Rankine-Hugoniot jump conditions can be obtained using

$$[\![\mathbf{F}(\boldsymbol{W})]\!] = S\,[\![\boldsymbol{W}]\!]\,.$$

This results in

$$\begin{aligned}
\rho(u-S)\,[\![\alpha_1]\!] &= 0,\\
[\![\alpha_1\rho_1(u_1-S)]\!] &= 0,\\
[\![\rho(u-S)]\!] &= 0,\\
-\alpha_1 Q_1\,[\![u_1]\!] + [\![\alpha_1 p_1]\!] - \alpha_2 Q_2\,[\![u_2]\!] + [\![\alpha_2 p_2]\!] &= 0,\\
\left[\!\!\left[\frac{1}{2}(u_1-S)^2 + \Psi_1\right]\!\!\right] - \left[\!\!\left[\frac{1}{2}(u_2-S)^2 + \Psi_2\right]\!\!\right] &= 0.
\end{aligned}$$

Shock Wave

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This results in

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[\![\alpha_1\rho_1(u_1-S)]\!] &= 0,\\
[\![\rho(u-S)]\!] &= 0,\\
-\alpha_1 Q_1\,[\![u_1]\!] + [\![\alpha_1 p_1]\!] - \alpha_2 Q_2\,[\![u_2]\!] + [\![\alpha_2 p_2]\!] &= 0,\\
\left[\!\!\left[\frac{1}{2}(u_1-S)^2+\Psi_1\right]\!\!\right] - \left[\!\!\left[\frac{1}{2}(u_2-S)^2+\Psi_2\right]\!\!\right] &= 0.
\end{aligned}$$

The jump conditions can be used to obtain the energy inequality across a discontinuity in a compact form

$$0 \geq -Q\left[\!\!\left[\Psi_1+\frac{1}{2}\,(u_1-S)^2\right]\!\!\right] \quad \text{or} \quad 0 \geq -Q\left[\!\!\left[\Psi_2+\frac{1}{2}\,(u_2-S)^2\right]\!\!\right].$$

Relation to the Baer-Nunziato Model

It is of further interest to compare the system (1) with the Baer-Nunziato model given by the following equations

$$
\begin{aligned}
\partial_t \alpha_1 + u_I \partial_x \alpha_1 &= \zeta_1, \\
\partial_t (\alpha_1 \rho_1) + \partial_x (\alpha_1 \rho_1 u_1) &= \zeta_2, \\
\partial_t (\alpha_2 \rho_2) + \partial_x (\alpha_2 \rho_2 u_2) &= \zeta_3, \\
\partial_t (\alpha_1 \rho_1 u_1) + \partial_x \left(\alpha_1 \rho_1 u_1^2 + \alpha_1 p_1(\rho_1) \right) - p_I \partial_x \alpha_1 &= \zeta_4, \\
\partial_t (\alpha_2 \rho_2 u_2) + \partial_x \left(\alpha_2 \rho_2 u_2^2 + \alpha_2 p_2(\rho_2) \right) - p_I \partial_x \alpha_2 &= \zeta_5.
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$$

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It is possible to show equivalence in the smooth case for

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u_I = u, \quad p_I = \frac{\alpha_2 \rho_2 p_1 + \alpha_1 \rho_1 p_2}{\rho}
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Differences in the presence of discontinuities!

Examples

Shock in Rarefaction

The following computation was performed using the ideal gas EOS

$$p_i(\rho_i) = \rho_i^{\gamma_i},\ i \in \{1, 2\} \quad \text{with} \quad \gamma_1 = 1.4,\ \gamma_2 = 2$$

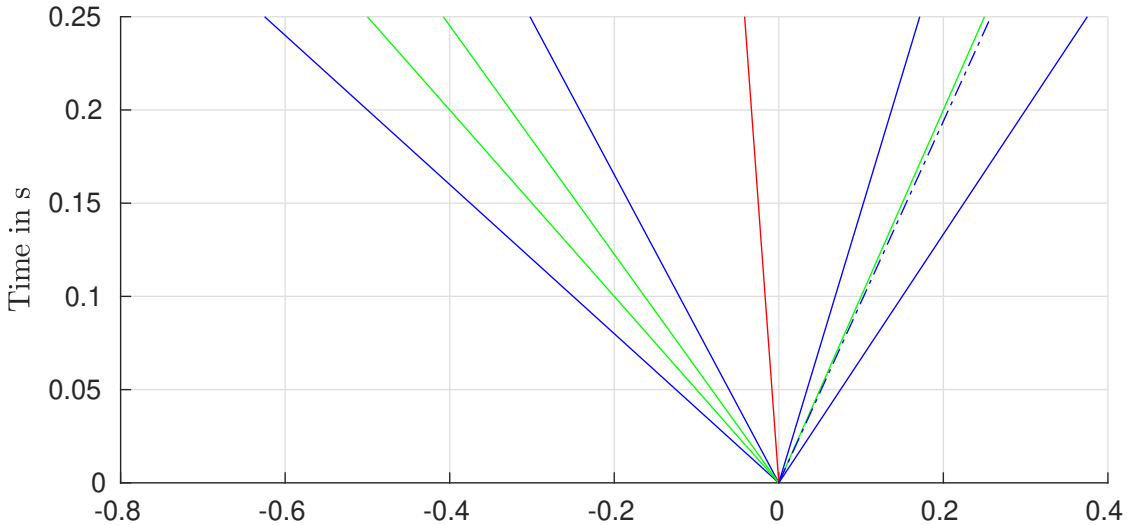
and the parameters

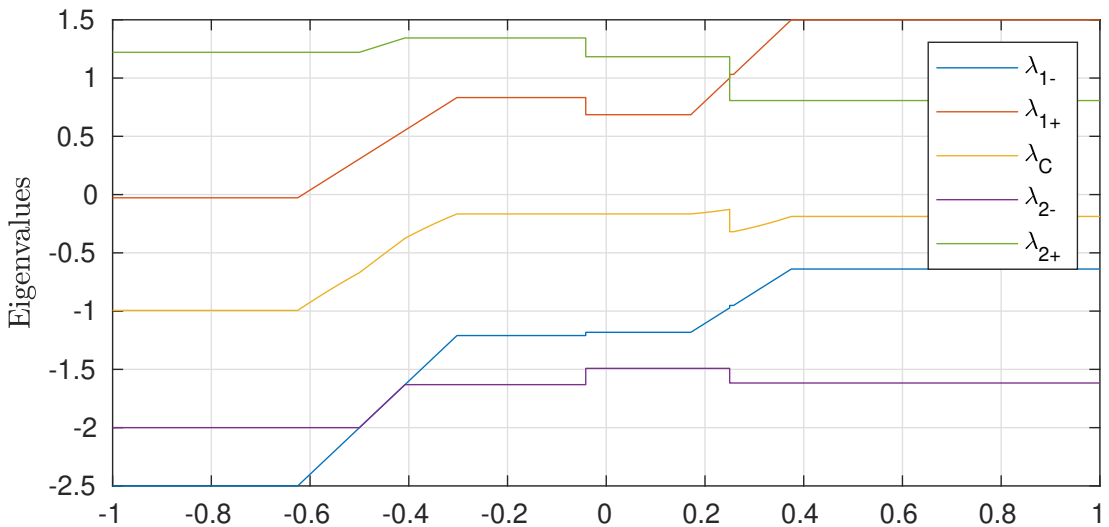
$$\Delta x = 0.5 \cdot 10^{-4}\,\text{m},\ C_{CFL} = 0.25,\ t_{end} = 0.25\,\text{s} \quad \text{and} \quad x \in [-1, 1]\,\text{m}.$$

For the numerical solution we used the Rusanov Flux together with Godunov's method as exemplary shown in[12].

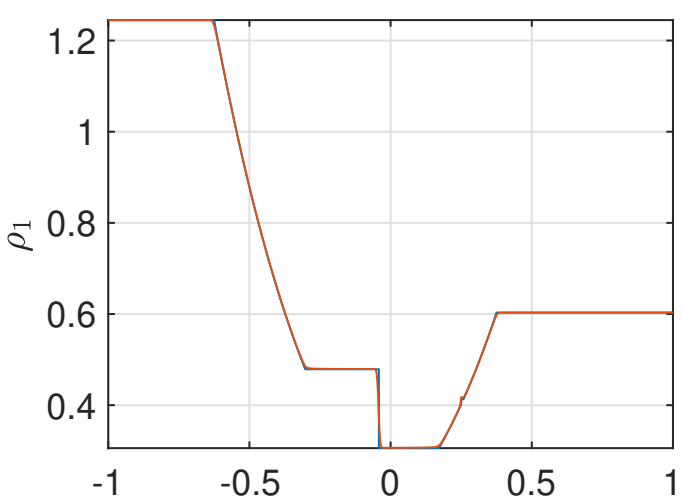
[12] Toro, E. F. *Riemann Solvers and Numerical Methods for Fluid Dynamics.* (Springer Berlin Heidelberg, 2009).

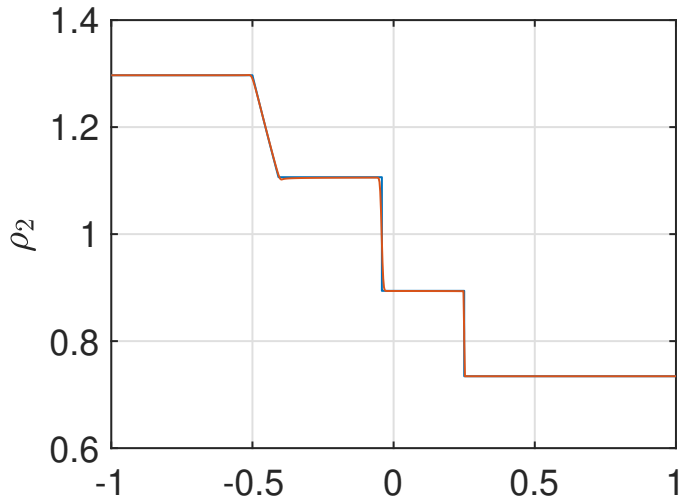
Shock in Rarefaction

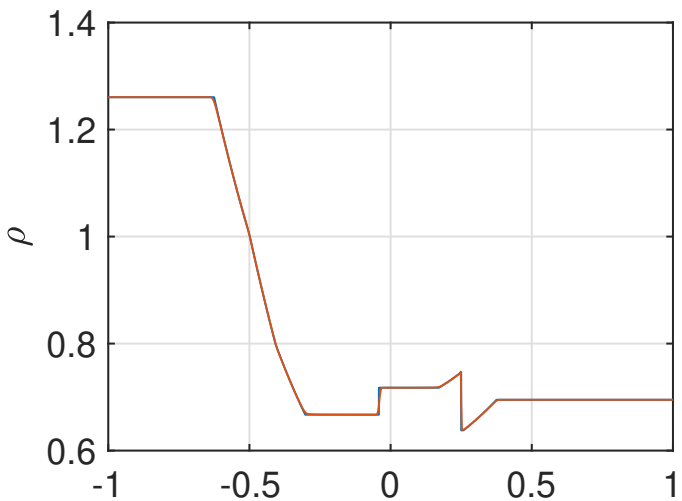


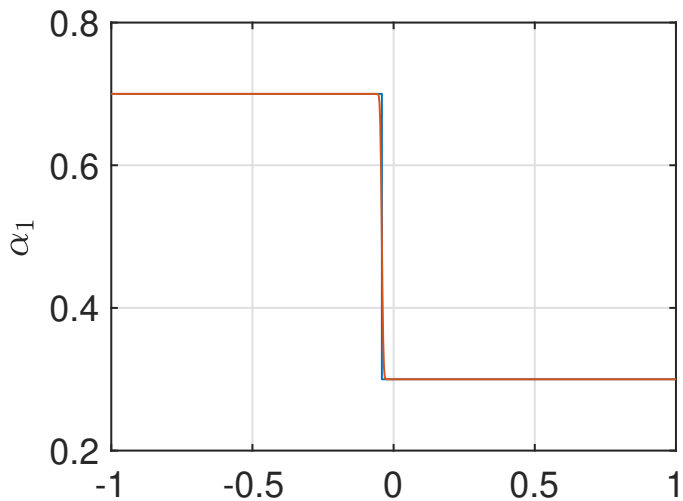


Shock in Rarefaction

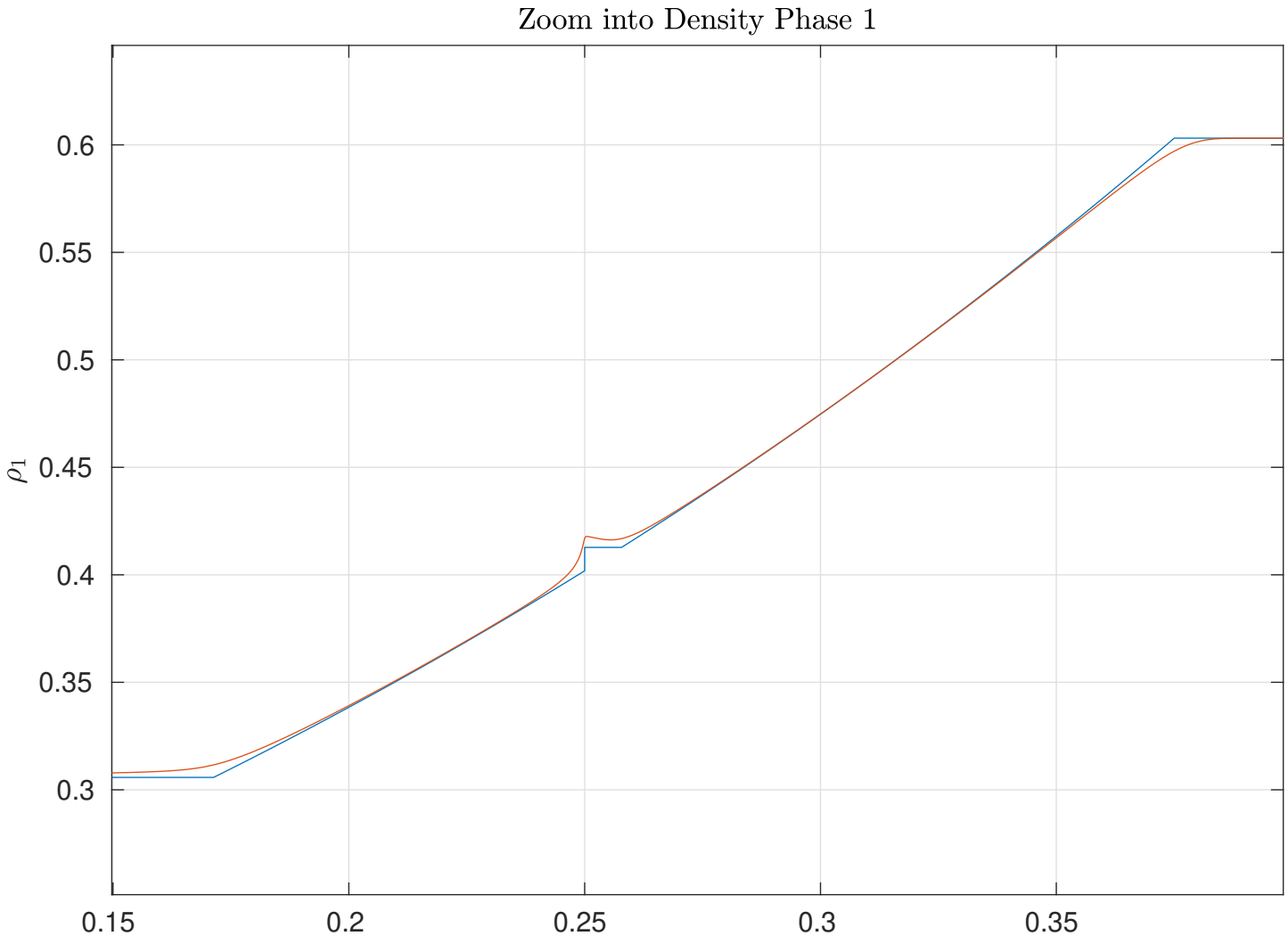




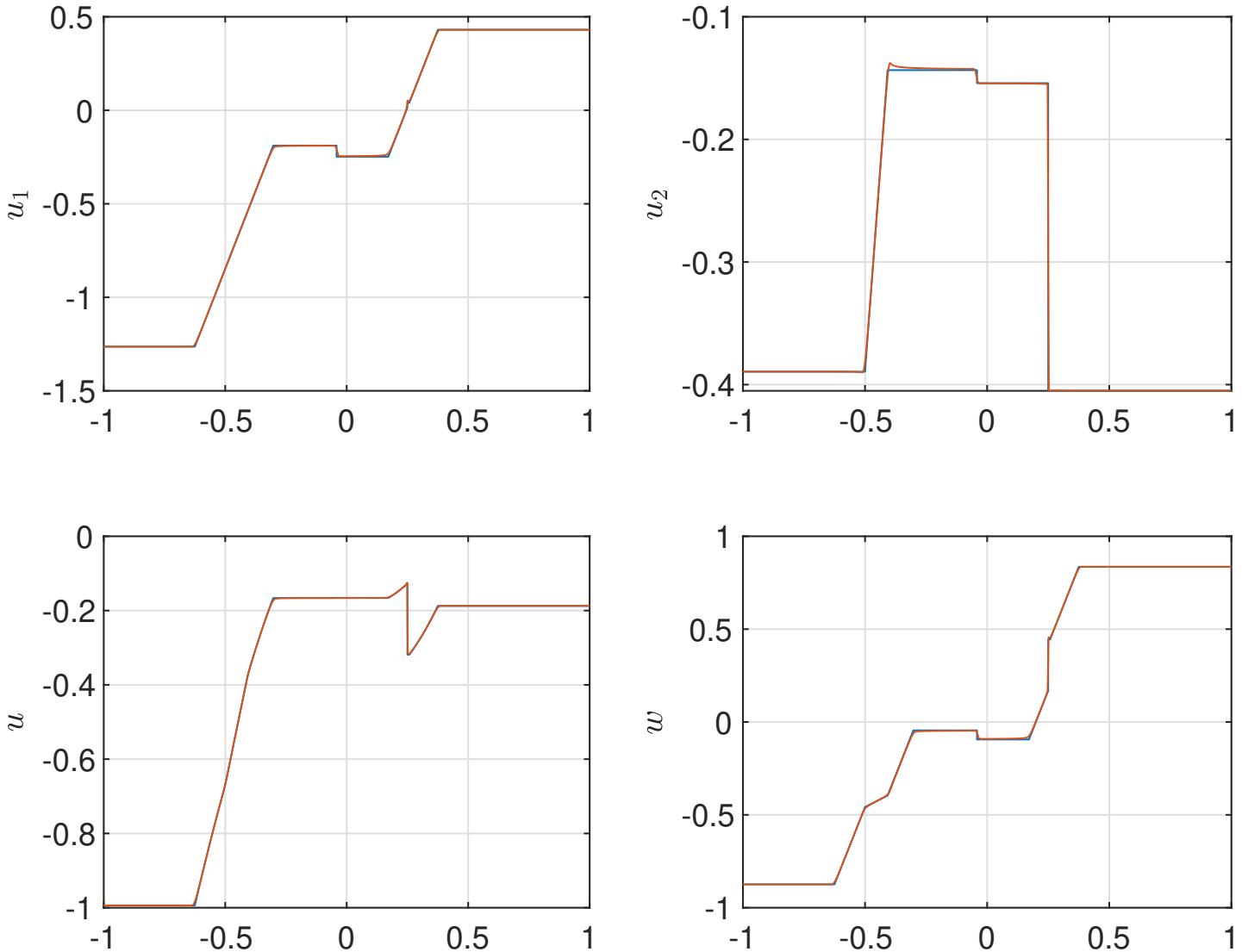




Shock in Rarefaction



Shock in Rarefaction



Comparison with Baer-Nunziato

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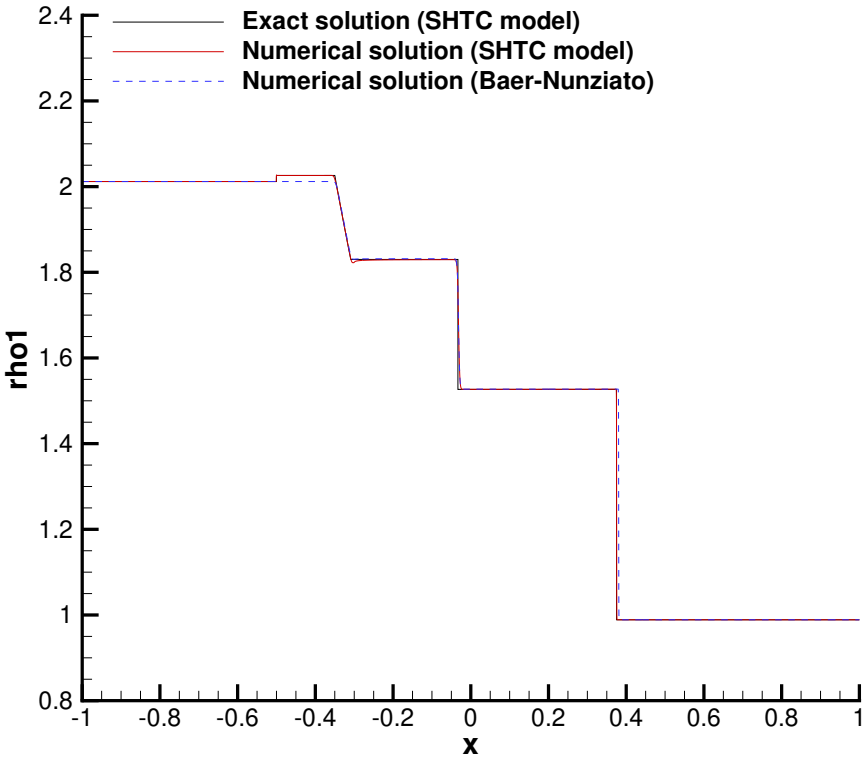
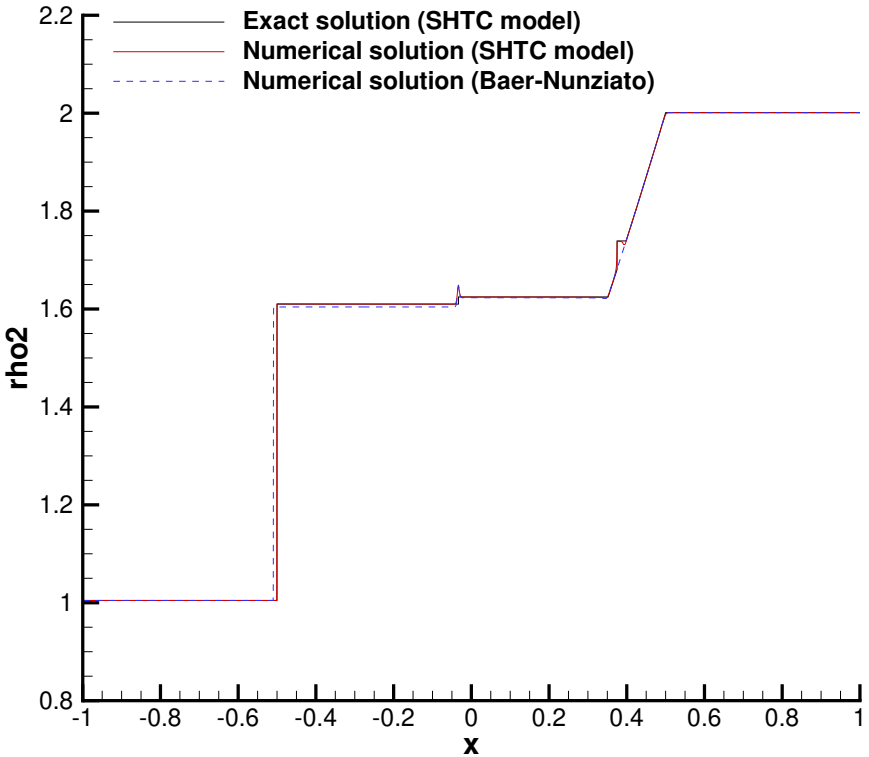
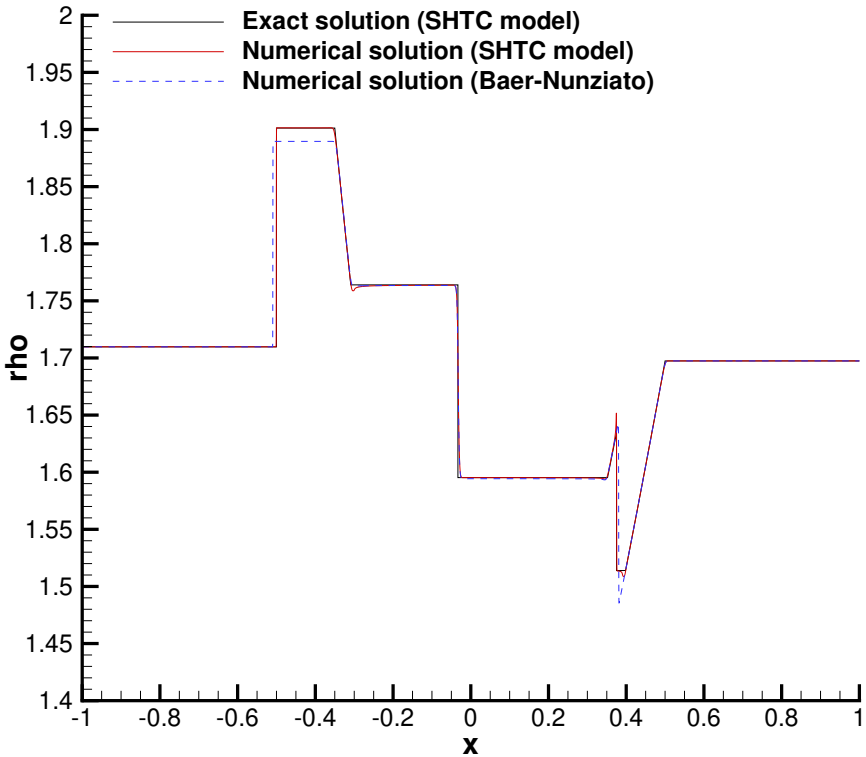
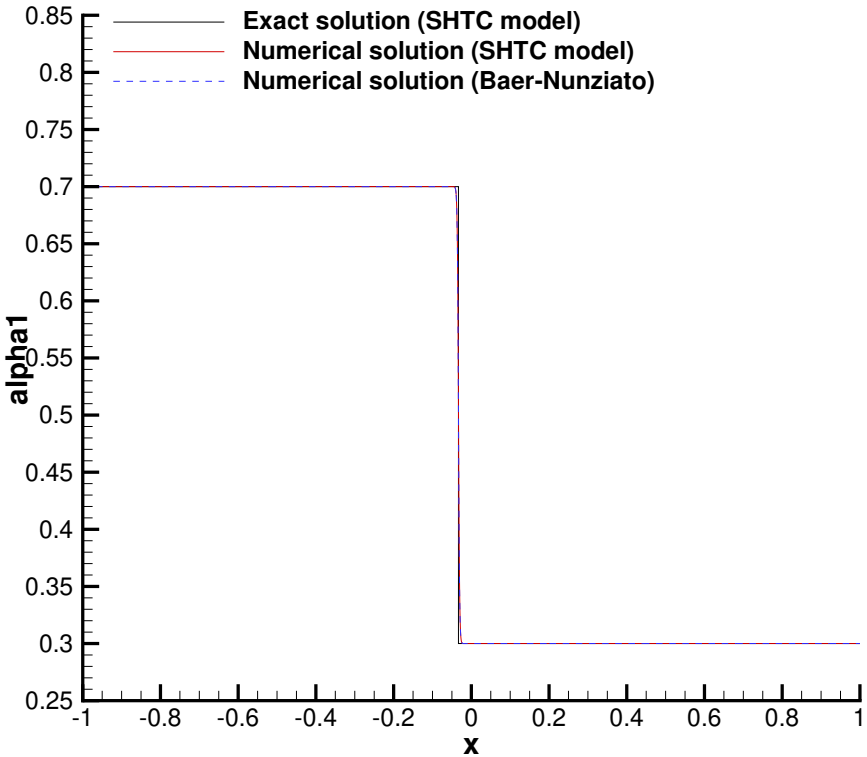




(a) Densities ρ_1, ρ_2.

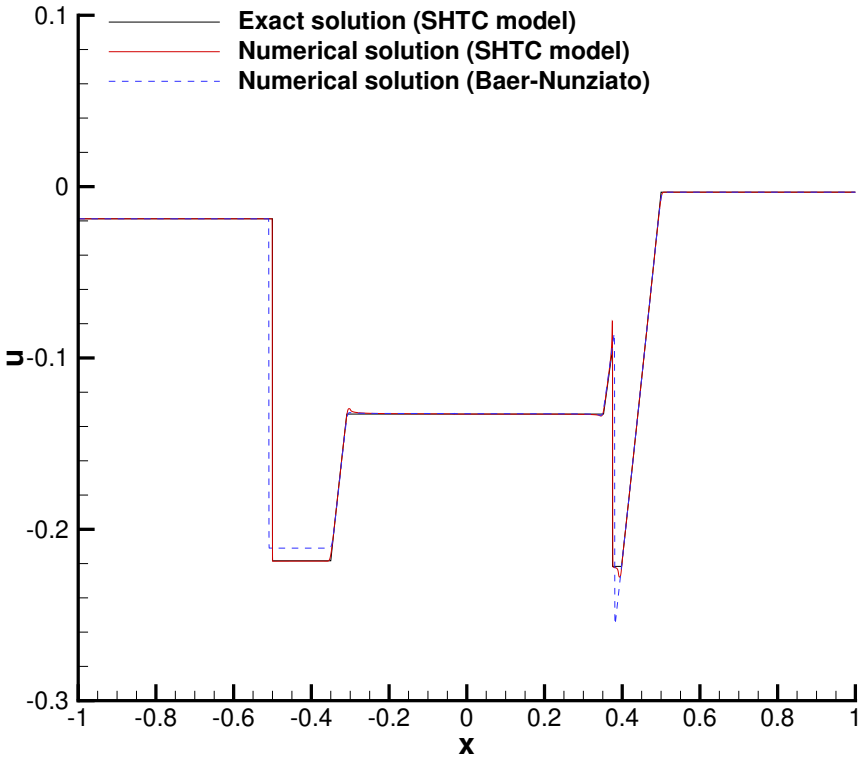
Comparison with Baer-Nunziato

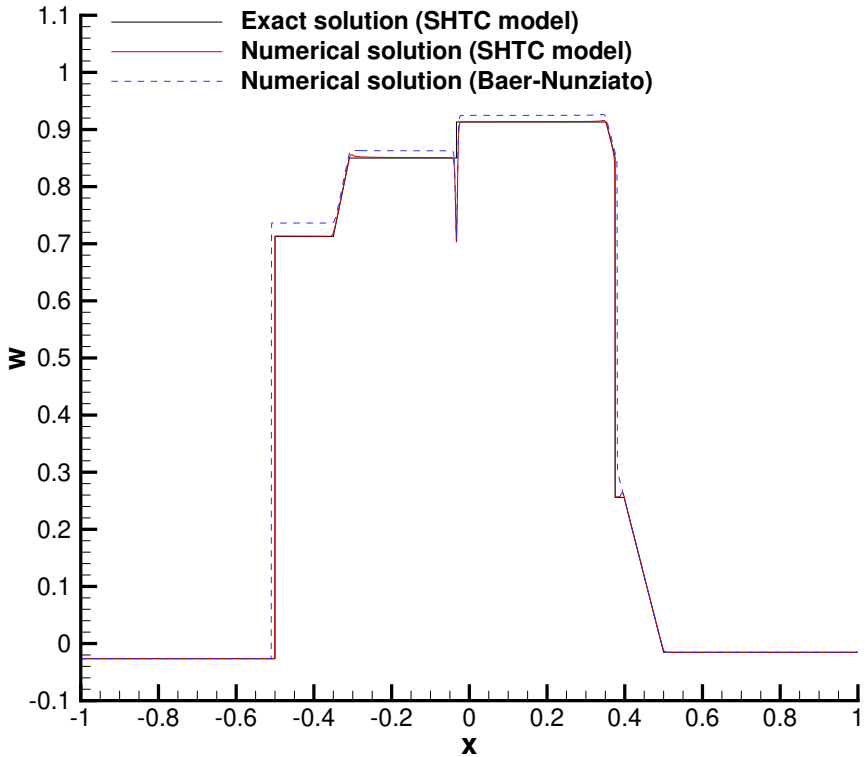




(b) Density ρ and volume fraction α_1.

Comparison with Baer-Nunziato





(c) Velocities u, w.

Key features:

1. non–strictly hyperbolic system
2. eigenvalues may coincide and change their ordering
3. characteristic fields *do not* change their character
4. shock in one phase influences the other phase
5. smooth solutions are a superposition of phase individual solutions
6. no vanishing of eigenvectors which belong to genuine non–linear fields
7. resonance may occur if α is constant in space
8. smooth equivalence to the barotropic Baer - Nunziato system

Future Work

- relation between different models
- investigate implications for the non–conservative system
- common test cases
- multi–dimensional analysis and numerics
- study prototype model to understand new wave phenomena
- ...

Thank you for your attention!

This work was supported by DFG - Grant 525939417
A sharp interface limit by vanishing volume fraction for non-equilibrium two phase flows modeled by hyperbolic systems of balance laws